Variational Methods for Latent Variable Problems

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Oct, 2021

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Outline

Outline for today:

- Some examples of latent variable models
- A template: The Neyman-Scott "paradox" and marginalization
- Bayesian versus frequentist approaches to marginalization
- The classical EM algorithm
- The EM algorithm as variational inference

Next week, we will build on these ideas to present more general variational inference.

Latent variable models: Microcredit effectiveness

Randomized controlled trials were run in seven different countries to measure the effect of access to microcredit on business profits. In each country, thousands of businesses were observed. These businesses share common, unobserved attributes of their particular country. [Meager, 2020]

The different levels of profit and microcredit effectiveness in each country are latent variables. We wish to infer the overall average effectiveness of microcredit, which is common to all observations.

Latent variable models: Mouse geonmics

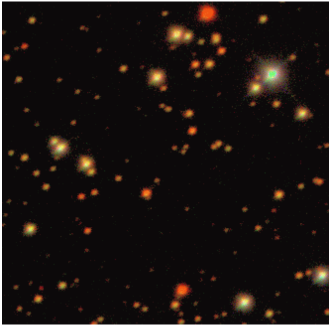
A set of mice were infected with an influenza virus, and the expression level for a large number of genes were measured over time. We wish to cluster together genes that have similarly shaped expression time series. [Luan and Li, 2003]

The cluster identities (archetypical time series of expression levels) are common to all observations. Which cluster a particular gene belongs to is a latent variable.

Latent variable models: Astronomical catalogs

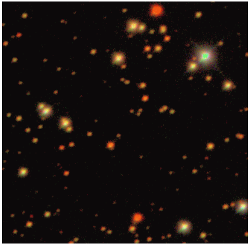
The Sloan Digital Sky Survey systematically photographed the night sky from the earth's surface. Astronomers wish to create a catalog of stars and galaxies and their properties that can be searched through and analyzed statistically, e.g. for evidence of dark matter. [Regier et al., 2019]

Each individual image contains distortion from that particular night's atmosphere and telescope configuration. The shape and identity of the astronomical objects are latent variables, and the distortion is common to all astronomical objects in a particular image. The typical shape and variability of the distortion is common to all images.



Latent variable models





Each of these models exhibits

- High dimensional "local" latent structure
- Low-dimensional "global" parameters of primary interest
- Possibly complicated dependence between the two (knowledge of the local variables informs the value of the globals, and vice-versa)

The Neyman-Scott "paradox"


...or why don't we always use the maximum likelihood estimator?

Here's a toy model. For some unknown z_n and θ, draw

$$y_{na}|z_n, \theta \sim \mathcal{N}(z_n, \theta)$$
$$y_{nb}|z_n, \theta \sim \mathcal{N}(z_n, \theta)$$

$$\text{Observations: } y = (y_{11}, y_{1b}, \ldots, y_{Na}, y_{Nb})$$
$$\text{Unknown latent variables: } z = (z_1, \ldots, y_N)$$
$$\text{Unknown global parameter: } \theta \in \mathbb{R}$$

Task: infer θ.

The Neyman-Scott "paradox"

$$y_{na}|z_n, \theta \sim \mathcal{N}(z_n, \theta) \qquad y_{nb}|z_n, \theta \sim \mathcal{N}(z_n, \theta)$$

Let's use that old workhorse, the maximum likelihood estimator (MLE)!

(**Spoiler:** Something will go wrong.)

The normal distribution gives (up to constants):

$$\log p(y_{na}, y_{nb}|\theta, z_n) = -\frac{1}{2}\theta^{-1}(y_{na} - z_n)^2 - \frac{1}{2} log\theta \quad -\frac{1}{2}\theta^{-1}(y_{nb} - z_n)^2 - \frac{1}{2}\log\theta$$

$$\log p(y|\theta, z) = \sum_{n=1}^{N} \log p(y_{na}, y_{nb}|\theta, z_n)$$

The MLE is given by:

$$\hat{\theta}, \hat{z} := \underset{\theta, z}{\mathrm{argmax}} \log p(y|\theta, z) \qquad \Leftrightarrow \qquad \left.\frac{\partial \log p(y|\theta, z)}{\partial(\theta, z)}\right|_{\hat{\theta}, \hat{z}} = 0$$

Exercise: Find an expression for $\hat{z}_n$.

The Neyman-Scott "paradox"

Exercise: Find an expression for $\hat{z}_n$.

$$
\begin{aligned}
0 &= \left.\frac{\partial \log p(y|\theta, z)}{\partial z_n}\right|_{\hat{z},\hat{\theta}} \\
&= \left.\frac{\partial \log p(y_{na}, y_{nb}|\theta, z_n)}{\partial z_n}\right|_{\hat{z},\hat{\theta}} \\
&= \left.\frac{\partial}{\partial z_n}\left(-\frac{1}{2}\theta^{-1}\left(y_{na} - z_n\right)^2 - \frac{1}{2}\log\theta - \frac{1}{2}\theta^{-1}\left(y_{nb} - z_n\right)^2 - \frac{1}{2}\log\theta\right)\right|_{\hat{z},\hat{\theta}} \\
&= -\hat{\theta}^{-1}(y_{na} - \hat{z}_n) - \hat{\theta}^{-1}(y_{nb} - \hat{z}_n) \Rightarrow \\
\hat{z}_n &= \frac{1}{2}(y_{na} + y_{nb}).
\end{aligned}
$$

Wonderful! This is a very sensible expression, and it doesn't depend on $\hat{\theta}$.

Exercise: Using this result, find an expression for $\hat{\theta}$.

Hint: $(y_{na} - \hat{z}_n)^2 = (y_{nb} - \hat{z}_n)^2 = \frac{1}{4}\left(y_{na} - y_{nb}\right)^2$

The Neyman-Scott "paradox"

Exercise: Find an expression for $\hat{\theta}$.

Hint: $(y_{na} - \hat{z}_n)^2 = (y_{nb} - \hat{z}_n)^2 = \frac{1}{4}(y_{na} - y_{nb})^2$

$$
\begin{aligned}
0 &= \left.\frac{\partial \log p(y|\theta, z)}{\partial \theta}\right|_{\hat{z},\hat{\theta}} \\
&= \frac{\partial}{\partial \theta} \sum_{n=1}^{N} \left.\left(-\frac{1}{2}\theta^{-1}(y_{na} - z_n)^2 - \frac{1}{2}\log\theta - \frac{1}{2}\theta^{-1}(y_{nb} - z_n)^2 - \frac{1}{2}\log\theta\right)\right|_{\hat{z},\hat{\theta}} \\
&= \sum_{n=1}^{N} \left(\frac{1}{2}\hat{\theta}^{-2}\frac{1}{4}(y_{na} - y_{nb})^2 - \frac{1}{2}\hat{\theta}^{-1} + \frac{1}{2}\hat{\theta}^{-2}\frac{1}{4}(y_{na} - y_{nb})^2 - \frac{1}{2}\hat{\theta}^{-1}\right) \\
&= \hat{\theta}^{-2}\frac{1}{4}\sum_{n=1}^{N}(y_{na} - y_{nb})^2 - N\hat{\theta}^{-1} \Rightarrow \\
\hat{\theta} &= \frac{1}{4}\frac{1}{N}\sum_{n=1}^{N}(y_{na} - y_{nb})^2 .
\end{aligned}
$$

Exercise: Suppose the true parameters are θ_0 and z_0.

What is the behavior of $\hat{\theta}$ for large N?

Hint: Use the law of large numbers.

The Neyman-Scott "paradox"

Exercise: What is the behavior of $\hat{\theta}$ for large N? By the law of large numbers,

$$\begin{aligned}
\hat{\theta} &= \frac{1}{4}\frac{1}{N}\sum_{n=1}^{N}(y_{na} - y_{nb})^2 \\
&\xrightarrow[N\to\infty]{prob} \frac{1}{4}\mathop{\mathbb{E}}_{p(y|\theta_0,z_0)}\left[(y_{na} - y_{nb})^2\right] \\
&= \frac{1}{4}\mathop{\mathbb{E}}_{p(y|\theta_0,z_0)}\left[(y_{na} - z_{0n} - (y_{nb} - z_{0n}))^2\right] \\
&= \frac{1}{4}\Bigg(\mathop{\mathbb{E}}_{p(y|\theta_0,z_0)}\left[(y_{na} - z_{0n})^2\right] + \mathop{\mathbb{E}}_{p(y|\theta_0,z_0)}\left[(y_{nb} - z_{0n})^2\right] + \\
&\qquad\qquad 2\mathop{\mathbb{E}}_{p(y|\theta_0,z_0)}\left[(y_{na} - z_{0n})(y_{nb} - z_{0n})\right]\Bigg) \\
&= \frac{1}{4}(\theta_0 + \theta_0 + 0) \\
&= \frac{\theta_0}{2} \neq \theta_0.
\end{aligned}$$

$\Rightarrow$ **The MLE is inconsistent. What went wrong?**

The Neyman-Scott "paradox"

The MLE is inconsistent. What went wrong?

$$\hat{z}_n = \frac{1}{2}(y_{na} + y_{nb})$$

$$\hat{\theta} \xrightarrow[N\to\infty]{prob} \frac{\theta_0}{2} \neq \theta_0$$

- Our estimates for the latent variables $\hat{z}_n$ are quite uncertain (they use only two observaitons each)
- But our MLE estimate for $\hat{\theta}$ treated the $\hat{z}_n$ as if they were known exactly
- $\Rightarrow$ We estimated less dispersion around $\hat{z}_n$ than was truly present. That is, we *under-estimated* the dispersion θ_0.
- To avoid this problem, we must *account for the uncertainty* in z_n when estimating θ.

Solution: **Marginalization.**

The Neyman-Scott "paradox"

To marginalize we must:

- Add a distributional assumption $z|\theta \sim p(z|\theta)$.
- Compute the marginal $p(y|\theta) = \int p(y|\theta, z)p(z|\theta)dz$.
- Compute the marginal MLE $\hat{\theta} = \mathrm{argmax}\,\theta p(y|\theta)$
  - (Contrast with $\hat{\theta}, \hat{z} = \mathrm{argmax}_{\theta,z}\, p(y|\theta, z)$)

Neyman-Scott resolved

Let's let $z_n \sim \mathcal{N}(0, 1)$. Then, by standard properties of the normal,

$$\begin{pmatrix} y_{na} \\ y_{nb} \end{pmatrix} \overset{iid}{\sim} \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1+\theta & 1 \\ 1 & 1+\theta \end{pmatrix}\right)$$

Sample covariances of the bivariate normal are consistent, so

$$\hat{\theta} := \underset{\theta}{\mathrm{argmax}} \sum_{n=1}^{N} \log \int p(y_{na}, y_{nb}|\theta, z_n)p(z_n)dz_n$$

is consistent.

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Jeffrey Regier, Keno Fischer, Kiran Pamnany, Andreas Noack, Jarrett Revels, Maximilian Lam, Steve Howard, Ryan Giordano, David Schlegel, Jon McAuliffe, et al. Cataloging the visible universe through bayesian inference in julia at petascale. *Journal of Parallel and Distributed Computing*, 127:89–104, 2019.